

Doubly constrained bounds on the entanglement of formation

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We derive bounds on the entanglement of formation of states of a $4 \times N$ bipartite system using two entanglement monotones constructed from operational separability criteria. The bounds are used simultaneously as constraints on the entanglement of formation. One monotone is the negativity, which is based on the Peres positive-partial-transpose criterion. For the other, we formulate a monotone based on a separability criterion introduced by Breuer (H.-P. Breuer, e-print quant-ph/0605036).

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The nonclassical correlations of entangled quantum states [1] have been of interest since the very inception of quantum mechanics [2, 3]. Quantum information science has led to the idea that entanglement is a resource for information processing and other tasks. The ability of quantum computers to solve classically hard problems efficiently, the increased security of quantum cryptographic protocols, and the enhanced capacity of quantum channels—all these are attributed to entanglement. Investigating entanglement has led to new understanding of techniques such as the density-matrix renormalization group [4] and of quantum phase transitions [5, 6] and properties of condensed systems [7]. Despite the importance of entanglement, however, characterizing and quantifying it in most physical systems that are of interest from an experimental standpoint remains a challenge.

An important measure of entanglement for a pure state $|\Psi\rangle$ of two systems, A and B , is the entropy, $-\text{Tr}(\rho_A \log \rho_A)$, of the marginal density operator ρ_A . We write this entropy sometimes as a function $h(\Psi)$ and sometimes as the Shannon entropy $H(\boldsymbol{\mu})$ of the vector $\boldsymbol{\mu}$ of Schmidt coefficients of $|\Psi\rangle$. This measure can be applied to bipartite mixed states by the convex-roof extension of $h(\Psi)$. The extended quantity, called the *entanglement of formation* (EOF), is defined as

$$h(\rho) \equiv \min_{\{p_j, |\Psi^j\rangle\}} \left\{ \sum_j p_j h(\Psi^j) \mid \rho = \sum_j p_j |\Psi^j\rangle\langle\Psi^j| \right\}. \quad (1)$$

The EOF is a *nonoperational* measure of entanglement because the minimization over all pure-state decompositions of ρ generally means there is no efficient procedure for calculating it. This minimization is the bottleneck in evaluating most nonoperational entanglement measures for mixed states. Consequently, bounding the EOF, instead of computing its value, becomes important.

An alternate approach to quantifying entanglement is based on the use of positive (but not completely positive) maps on density operators [8]. A quantum state is *separable* if and only if it remains positive semidefinite under the action of *any* positive map. Given a positive map, we can construct a related entanglement monotone by

considering the spectrum of density operators under the action of the map [9, 10]. Such monotones are typically much easier to calculate for general quantum states, because they do not involve the convex-roof construction, and thus are said to be *operational* [1].

We can use the monotones constructed from positive maps and from other operational entanglement criteria as constraints to obtain bounds on nonoperational, convex-roof extended measures of entanglement. The complexity of the minimization in Eq. (1) is reduced by solving it over a constrained set, instead of over all pure-state decompositions. This was done in [11, 12] for the EOF, using a single operational constraint. Our endeavor in this Letter is to carry this program forward. We first sketch a general scheme for many constraints, which we discuss further in [13], and then illustrate the general scheme for a particular case of two operational constraints.

Let us say that f_1, \dots, f_K are operational entanglement monotones for a bipartite system. We gather their values for an arbitrary state ρ into a vector $\mathbf{n} = (n_1, \dots, n_K)$. Their actions on pure states are functions of the Schmidt coefficients, i.e., $f_k(\Psi) = F_k(\boldsymbol{\mu})$ for $k = 1, \dots, K$.

We are interested in a lower bound on the value of the EOF. Let us assume that for the state ρ , the optimal pure-state decomposition is $\rho = \sum_j p_j |\Psi^j\rangle\langle\Psi^j|$, giving $h(\rho) = \sum_j p_j H(\boldsymbol{\mu}^j)$. Now define the function

$$\tilde{H}(\mathbf{m}) = \min_{\boldsymbol{\mu}} \left\{ H(\boldsymbol{\mu}) \mid F_k(\boldsymbol{\mu}) = m_k, k = 1, \dots, K \right\}. \quad (2)$$

Notice that $\tilde{H}(\mathbf{m})$ is defined only on the region of possible values of \mathbf{m} corresponding to pure states, a region we call the *pure-state region*. If \tilde{H} is not a monotonically nondecreasing function of \mathbf{m} , which we will call a monotonic function for brevity, we replace it with such a monotonic function $\tilde{H}_\uparrow(\mathbf{m})$, constructed by dividing the pure-state region into subregions on which subsets of the constraints are applied. We describe the procedure for constructing $\tilde{H}_\uparrow(\mathbf{m})$ in detail in [13].

Let $\mathcal{H}(\mathbf{m}) = \text{co}[\tilde{H}_\uparrow(\mathbf{m})]$ be the convex hull of $\tilde{H}_\uparrow(\mathbf{m})$, i.e., the largest convex function of K variables

(m_1, \dots, m_K) bounded from above by $\tilde{H}_1(\mathbf{m})$. We can show that $\mathcal{H}(\mathbf{m})$ is also a monotonic function [13], which can be extended naturally to a monotonic function on the entire space of values of \mathbf{m} . Using Eq. (2) and the convexity and monotonicity of \mathcal{H} , we can write

$$h(\rho) \geq \sum_j p_j \mathcal{H}(\mathbf{n}^j) \geq \mathcal{H}\left(\sum_j p_j \mathbf{n}^j\right) \geq \mathcal{H}(\mathbf{n}), \quad (3)$$

where we have used the convexity of the monotones f_k to obtain $\sum_j p_j n_k^j \geq n_k$. Knowing the easily calculated \mathbf{n} for ρ thus leads to a bound on $h(\rho)$.

We now carry through the general program for $4 \times N$ states using two operational entanglement monotones as constraints. Ours is the first instance of a doubly constrained bound on an entanglement measure for a family of states. It gives tighter bounds than those obtained previously [11].

The first monotone is the *negativity* [10], which is based on the Peres criterion [14]. The negativity of a bipartite state ρ is defined as $n_T(\rho) = (\|\rho^{T_A}\| - 1)/2$ where T_A is the partial transposition with respect to system A and the trace norm is defined as $\|O\| = \text{Tr}(\sqrt{OO^\dagger})$. For pure states, the negativity, in terms of the Schmidt coefficients, is given by $n_T = [(\sum_j \sqrt{\mu_j})^2 - 1]/2$.

We define a second monotone based on the Φ -map introduced by Breuer [15]. The action of the Φ -map on any state σ is given by $\Phi(\sigma) = \text{Tr}(\sigma)I - \sigma - V\sigma^T V^\dagger$, where the superscript T stands for transposition and V is a unitary matrix with matrix elements $\langle j, m|V|j, m'\rangle = (-1)^{j-m}\delta_{m,-m'}$ in the angular momentum basis $\{|j, m\rangle\}$. The map Φ provides, for any bipartite state ρ having a subsystem with even dimension greater than 4, a non-trivial condition for separability as $(I \otimes \Phi)(\rho) \geq 0$. The related entanglement monotone, which we call the Φ -negativity, is defined for a general mixed state as

$$n_\Phi(\rho) = \frac{D(D-1)}{4} \left[\frac{\|(I \otimes \Phi)(\rho)\|}{D-2} - 1 \right], \quad (4)$$

where D is the dimension of the smaller of the two systems in the bipartite state ρ . The Φ -negativity is a convex function of ρ . For $4 \times N$ systems ($N \geq 4$), the Φ -negativity for pure states, as a function of the four Schmidt coefficients, is $n_\Phi = 3\sqrt{(\mu_1 + \mu_4)(\mu_2 + \mu_3)}$. The Φ -negativity for various states is given in [13].

We can place bounds on the EOF of $4 \times N$ states by using either n_Φ or n_T as constraints. To find the bound with n_T as the single constraint, which was done in [11], one first finds the singly constrained function $\tilde{H}(n_T)$ of Eq. (2). This function being monotonic, but not convex, its convex roof gives the bound. For the $4 \times N$ states we consider, the bound is given by

$$\mathcal{H}(n_T) = \begin{cases} H_2(\gamma) + (1-\gamma)\log_2 3, & n_T \in [0, 1], \\ (n_T - \frac{3}{2})\log_2 3 + 2, & n_T \in [1, \frac{3}{2}], \end{cases} \quad (5)$$

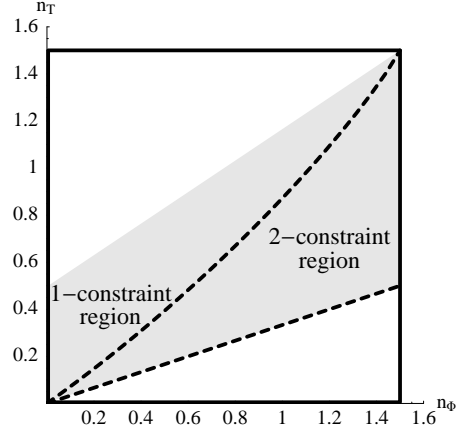


FIG. 1: The shaded region is the pure-state region in the n_Φ - n_T plane for $4 \times N$ pure states. The dashed lines are the monotone boundaries given by Eq. (8) and by $n_T = n_\Phi/3$. In the 2-constraint region between the monotone boundaries, we set $\tilde{H}_1(\mathbf{n}) = \tilde{H}(\mathbf{n})$, and in the 1-constraint region above the upper monotone boundary, we set $\tilde{H}_1(\mathbf{n}) = \tilde{H}(n_T)$.

where H_2 is the binary entropy function and $\gamma = (\sqrt{2n_T+1} + \sqrt{9-6n_T})^2/16$. If instead we use n_Φ as the single constraint, we first find the function $\tilde{H}(n_\Phi)$, which being monotonic and convex, gives directly a different bound on the EOF of $4 \times N$ states [13],

$$\tilde{H}(n_\Phi) = \mathcal{H}(n_\Phi) = H_2(\alpha), \quad \alpha = \frac{1 + \sqrt{1 - 4n_\Phi^2/9}}{2}. \quad (6)$$

We refer to $\mathcal{H}(n_\Phi)$ and $\mathcal{H}(n_T)$ as *singly constrained* bounds on the EOF. We now proceed to place a *doubly constrained bound* on the EOF of $4 \times N$ density operators by simultaneously using n_T and n_Φ as constraints.

Both n_Φ and n_T take on values between 0 and $3/2$, so all $4 \times N$ states lie in a square of side $3/2$ in the n_Φ - n_T plane. Not all points in the square correspond to pure states. Solving simultaneously the normalization constraint $\sum_{j=1}^4 \mu_j = 1$ and the two constraint equations, $\sum_{j=1}^4 \sqrt{\mu_j} = \sqrt{2n_T+1}$ and $3\sqrt{(\mu_1 + \mu_4)(\mu_2 + \mu_3)} = n_\Phi$, lets us express μ_1 , μ_2 , and μ_3 in terms of n_Φ , n_T , and μ_4 . For some values of n_Φ and n_T , there is no value for μ_4 for which the other three Schmidt coefficients are real numbers in the interval $[0, 1]$.

To find the pure-state region, we look for the maximum and minimum allowed values of n_T for a fixed n_Φ , assuming a pure state. To find the maximum, we apply the technique of Lagrange multipliers and obtain $n_T = 2n_\Phi/3 + 1/2$. The minimum lies on the boundary of allowed values of μ , with $\mu_3 = \mu_4 = 0$, and is given by $n_T = n_\Phi/3$. The resulting pure-state region, shown in Fig. 1, is convex. The pure-state region is not convex in general, however; the subtleties this introduces into our program are addressed in [13].

To find the doubly constrained bound on the EOF, we start with the function (2), specialized to our two

constraints,

$$\tilde{H}(n_\Phi, n_T) \equiv \min_{\boldsymbol{\mu}} \left\{ H(\boldsymbol{\mu}) \left| \sum_j \sqrt{\mu_j} = \sqrt{2n_T + 1}, \right. \right. \\ \left. \left. 3\sqrt{(\mu_1 + \mu_4)(\mu_2 + \mu_3)} = n_\Phi \right\}. \quad (7)$$

It turns out that $\tilde{H}(n_\Phi, n_T)$ is not monotonic, so we must replace it with the monotonic function $\tilde{H}_\uparrow(n_\Phi, n_T)$ discussed above. The procedure for constructing $\tilde{H}_\uparrow(n_\Phi, n_T)$, depicted in Fig. 1, makes a connection to the singly constrained bounds. This connection is based on the fact that the minimum of *any* function subject to two constraints is greater than or equal to the minimum of the same function subject to only one of the two constraints. Thus we can say that $\tilde{H}(n_\Phi, n_T) \geq \tilde{H}(n_T)$ for all n_Φ and $\tilde{H}(n_\Phi, n_T) \geq \tilde{H}(n_\Phi)$ for all n_T .

The minimum of $H(\boldsymbol{\mu})$ subject only to the n_T constraint, i.e., $\tilde{H}(n_T)$, occurs when the Schmidt coefficients are given by $\boldsymbol{\mu} = (\gamma, \gamma', \gamma', \gamma')$ [11] with $\gamma' = (1 - \gamma)/3$. This corresponds to $n_\Phi = \sqrt{2(2\gamma + 1)(1 - \gamma)}$, thus defining a curve in the n_Φ - n_T plane. Writing γ in terms of n_T puts this curve in the form

$$n_T = \frac{3}{4} \left(1 - \sqrt{1 - \frac{4}{9}n_\Phi^2} + \sqrt{\frac{4}{3}n_\Phi^2 + 2\sqrt{1 - \frac{4}{9}n_\Phi^2} - 2} \right). \quad (8)$$

Along this curve, which we call a *monotone boundary*, the n_Φ constraint is automatically satisfied when $H(\boldsymbol{\mu})$ is minimized with respect just to the n_T constraint, which means that $\tilde{H}(n_\Phi, n_T) = \tilde{H}(n_T)$ on this monotone boundary. To construct the required monotonic function, we set $\tilde{H}_\uparrow(n_\Phi, n_T) = \tilde{H}(n_T)$ when $n_\Phi \leq \sqrt{2(2\gamma + 1)(1 - \gamma)}$, i.e., above this monotone boundary.

Similarly, the minimum of $H(\boldsymbol{\mu})$ subject just to the n_Φ constraint, i.e., $\tilde{H}(n_\Phi)$, occurs when $\boldsymbol{\mu}_\Phi = (\alpha, 1 - \alpha, 0, 0)$, which gives a lower monotone boundary $n_T = \sqrt{\alpha(1 - \alpha)} = n_\Phi/3$. Along this line, the n_T constraint is automatically satisfied when $H(\boldsymbol{\mu})$ is minimized with respect just to the n_Φ constraint, which gives $\tilde{H}(n_\Phi, n_T) = \tilde{H}(n_\Phi)$ on this boundary. Since this lower monotone boundary coincides with the lower boundary of the pure-state region, it has no impact on defining $\tilde{H}_\uparrow(n_\Phi, n_T)$.

The definition of $\tilde{H}_\uparrow(\mathbf{n})$ is depicted in Fig. 1. Between the monotone boundaries, a region we call the *2-constraint region*, we set $\tilde{H}_\uparrow(\mathbf{n}) = \tilde{H}(\mathbf{n})$, and in the pure-state region above the upper monotone boundary, which we call the *1-constraint region*, we set $\tilde{H}_\uparrow(\mathbf{n}) = \tilde{H}(n_T)$. The resulting function $\tilde{H}_\uparrow(\mathbf{n})$ is monotonic throughout the pure-state region.

We now focus on finding $\tilde{H}(\mathbf{n})$ in the 2-constraint region. The method of Lagrange multipliers is not suitable for finding the minimum (7) because the problem is overconstrained. The equations obtained using Lagrange

multipliers have a consistent solution only if n_Φ and n_T are related as in Eq. (8), in which case $\tilde{H}(\mathbf{n}) = \tilde{H}(n_T)$. This does not mean that there is no minimum for $H(\boldsymbol{\mu})$ for other values of n_Φ and n_T , just that the minimum lies on a boundary of allowed values of $\boldsymbol{\mu}$. The boundary with three of the Schmidt coefficients being zero is the origin in the n_Φ - n_T plane, where $H(\boldsymbol{\mu}) = 0$. The boundary with two zero Schmidt coefficients is the line $n_T = n_\Phi/3$, and along this line $\tilde{H}(\mathbf{n}) = \tilde{H}(n_\Phi)$.

The minimum of $H(\boldsymbol{\mu})$ in the remaining part of the 2-constraint region can be found using a straightforward numerical procedure. As discussed above, the constraint equations can be solved to express μ_1, μ_2 , and μ_3 in terms of n_Φ, n_T , and μ_4 . There are two distinct solutions, $\boldsymbol{\mu}^{(1)}$ and $\boldsymbol{\mu}^{(2)}$. For a particular value of μ_4 , one or both of these solutions can be invalid in parts of the pure-state region because one or more of the three Schmidt coefficients lies outside the interval $[0, 1]$. For valid solutions we compute the entropy $H(\boldsymbol{\mu})$.

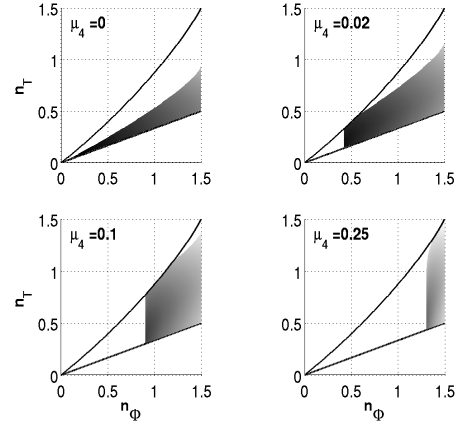


FIG. 2: The part of the 2-constraint region covered by four values of μ_4 . The two lines are the monotone boundaries.

We first consider the boundary where one Schmidt coefficient is zero by setting $\mu_4 = 0$ in the solutions $\boldsymbol{\mu}^{(1)}$ and $\boldsymbol{\mu}^{(2)}$. Not all points in the 2-constraint region can be reached if we set $\mu_4 = 0$. This is easily seen by noticing that the point $n_\Phi = n_T = 3/2$ corresponds uniquely to a maximally entangled $4 \times N$ state, and for this state all four Schmidt coefficients have the value $1/4$. Indeed, a continuum of points cannot be reached if we stay on the boundary defined by $\mu_4 = 0$, so we increase the value of μ_4 in small steps. The parts of the 2-constraint region that are covered by four values of μ_4 are shown in Fig. 2.

This numerical procedure gives us, for each point $\mathbf{n} = (n_\Phi, n_T)$ in the pure-state region, the range of values of μ_4 for which $H(\boldsymbol{\mu}^{(1)})$ and/or $H(\boldsymbol{\mu}^{(2)})$ can be calculated at that point. The minimum of these entropies over the allowed range of values for μ_4 is the value of $\tilde{H}(\mathbf{n})$.

The function $\tilde{H}(\mathbf{n})$ in the 2-constraint region is, as required, a monotonic function of both n_Φ and n_T . It is

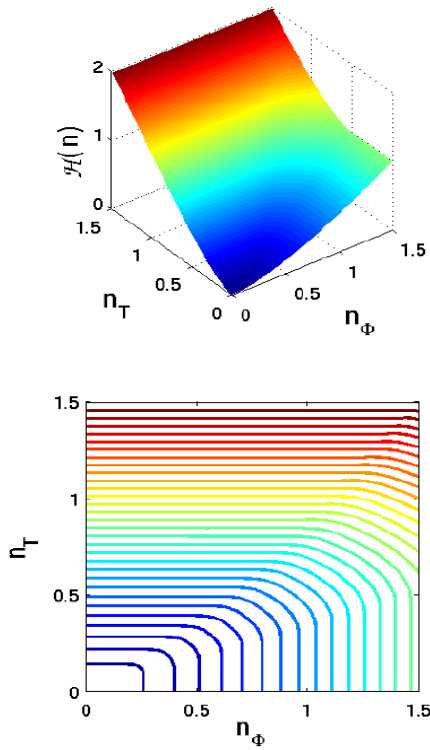


FIG. 3: (Color online) The doubly constrained bound $\mathcal{H}(\mathbf{n})$ on the EOF of $4 \times N$ states. Also shown is a contour plot of the same function.

extended to the monotonic function $\tilde{H}_\uparrow(\mathbf{n})$ on the entire pure-state region using the procedure outlined above. The monotonic function $\tilde{H}_\uparrow(\mathbf{n})$ is not convex, however, so we must compute its convex hull $\mathcal{H}(\mathbf{n})$. This can be done numerically, and it turns out that the difference between $\mathcal{H}(\mathbf{n})$ and $\tilde{H}_\uparrow(\mathbf{n})$ is quite small ($\sim 10^{-3}$), the two functions differing only in a small area near the maximally entangled state. Had the pure-state region, on which $\tilde{H}_\uparrow(\mathbf{n})$ is defined, not been convex, $\mathcal{H}(\mathbf{n})$ would be defined on an extended convex domain [13].

To obtain a bound on the EOF of *all* $4 \times N$ states, we have to extend $\mathcal{H}(\mathbf{n})$ outside the pure-state region to the rest of the n_Φ - n_T plane. The extension has to preserve the monotonicity of $\mathcal{H}(\mathbf{n})$ so that the string of inequalities in Eq. (3) holds. This is achieved by extending $\mathcal{H}(\mathbf{n})$ using surfaces that match the function at the lower and upper boundaries of the pure-state region. To preserve monotonicity, the surface added in the region below the lower boundary has zero slope along the n_T direction, and the surface added in the region above the upper boundary has zero slope along the n_Φ direction. The resulting doubly constrained bound $\mathcal{H}(\mathbf{n})$ on the EOF is shown in Fig. 3. The figure indicates that the extension to the whole n_Φ - n_T plane produces a smooth and seamless surface.

A third constraint based on the realignment criterion [16, 17] can be used to improve our bound on the EOF for certain classes of states. We can define the re-

alignment negativity for a bipartite density operator ρ as $n_R = (||\mathcal{R}(\rho)|| - 1)/2$, where $[\mathcal{R}(\rho)]_{ij,kl} = \rho_{ik,jl}$. For pure states, $n_R = n_T$. This means that in deriving the bounds, we could have redefined n_T as $\max(n_T, n_R)$.

In this Letter we focused on the derivation of a particular doubly constrained bound on the EOF of $4 \times N$ systems. Starting from the Φ -map introduced by Breuer [15, 18], we defined an entanglement monotone, the Φ -negativity, and combined it with the usual negativity to formulate a doubly constrained bound. We found that the pure-state region in the n_Φ - n_T plane is divided into sectors by monotone boundaries. The doubly constrained pure-state marginal entropy is applicable only in the region between the monotone boundaries. In the remaining portions of pure-state region, singly constrained entropies are applicable. Monotonicity and convexity dictate how to extend the bound to all states. We expect these features to persist for systems that are not $4 \times N$ and for more than two constraints, in which case the monotone boundaries will generally be hypersurfaces. A sector in which an m -constrained marginal entropy holds will be bounded by sectors in which $(m - 1)$ -constrained marginal entropies hold. These methods might provide a useful procedure for bounding the EOF and other convex-roof entanglement monotones.

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